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Title: DRACO and Nonequilibrium Statistical Mechanics of Aging

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DRACO and Nonequilibrium Statistical Mechanics of Aging

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Outline

- Types of problems which DRACO was designed to address

- Tools from nonequilibrium statistical mechanics:
- Rare events (Extreme value statistics)
- Transients (Diverging time scales)
- Thresholds (Absorbing phase transitions)

DRACO

- Multi-physics simulation
- Combines materials models with gas flow geometry

$$
\begin{cases}
A + X \xrightarrow{k_1} 2X & \text{(1)} \\
X + Y \xrightarrow{k_2} 2Y & \text{(2)} \\
Y \xrightarrow{k_3} B & \text{(3)}
\end{cases}
$$

+

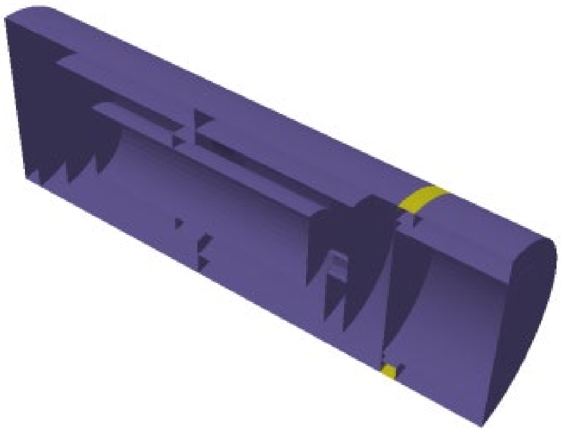
$$\frac{da(t)}{dt} = -k_1 a(t) x(t)$$

$$\frac{db(t)}{dt} = -k_2 b(t) y(t)$$

$$\frac{dx(t)}{dt} = -k_1 a(t) x(t) + k_2 b(t) y(t)$$

$$\frac{dy(t)}{dt} = k_1 a(t) x(t) - k_2 b(t) y(t)$$

+



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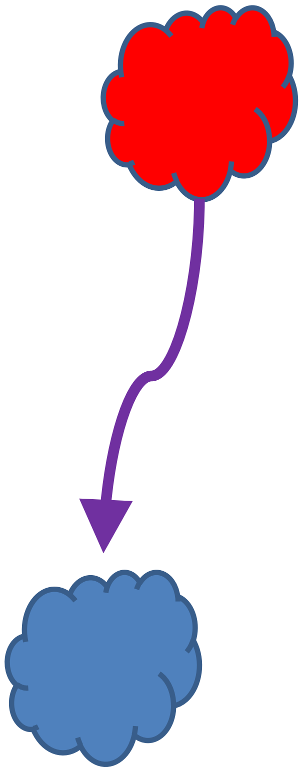
Gas flow



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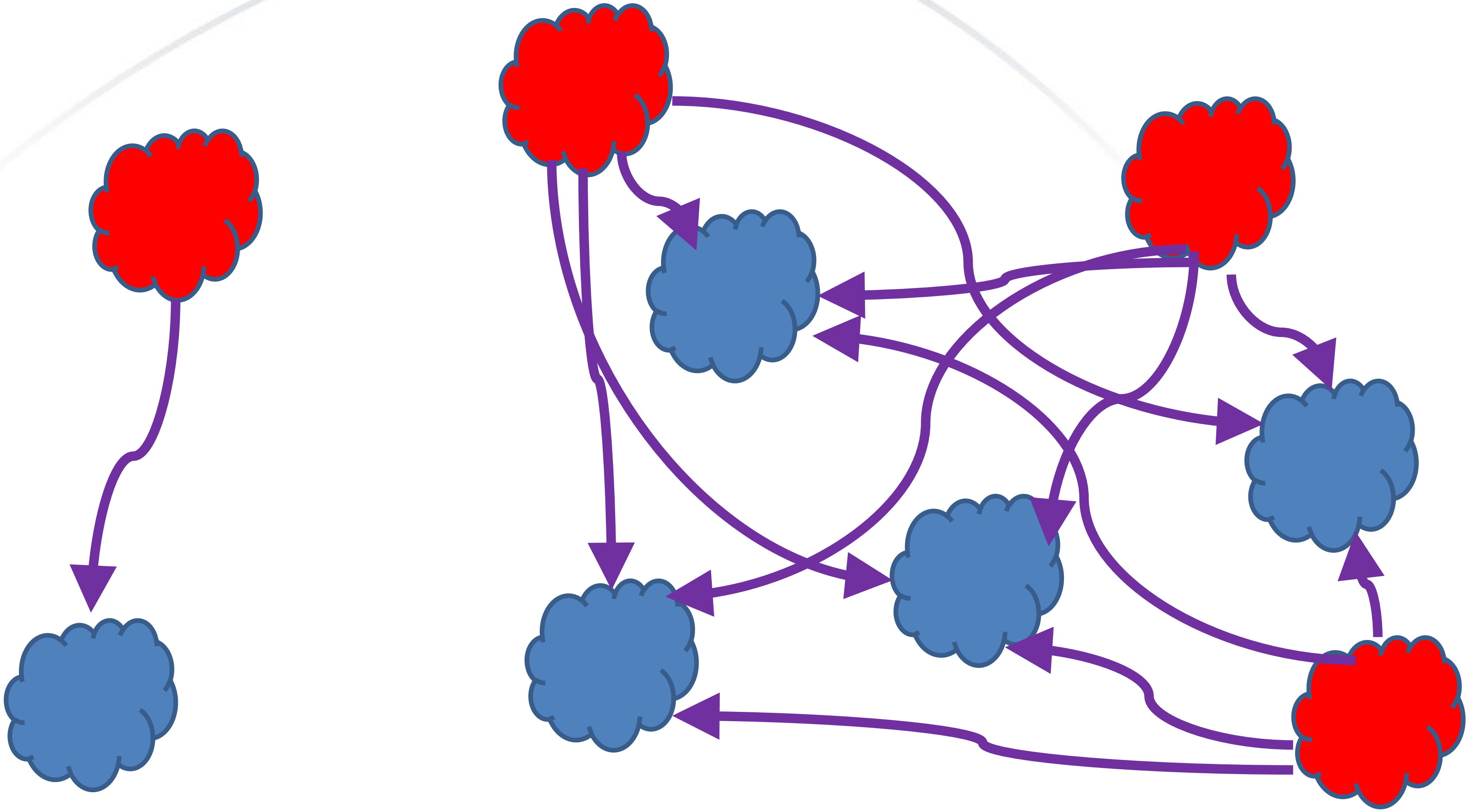
Gas flow



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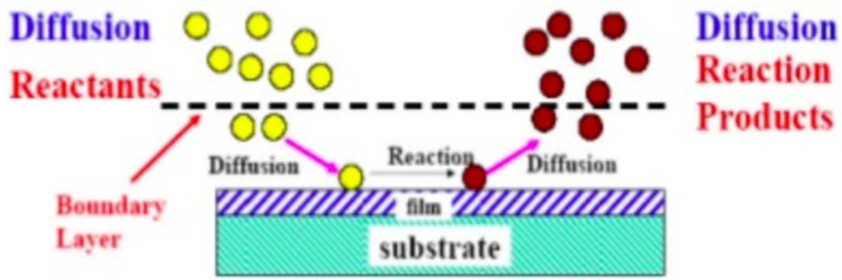
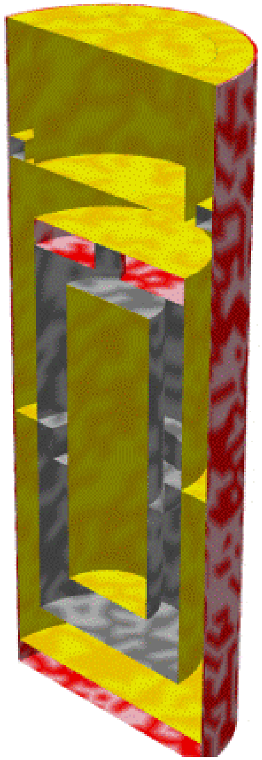
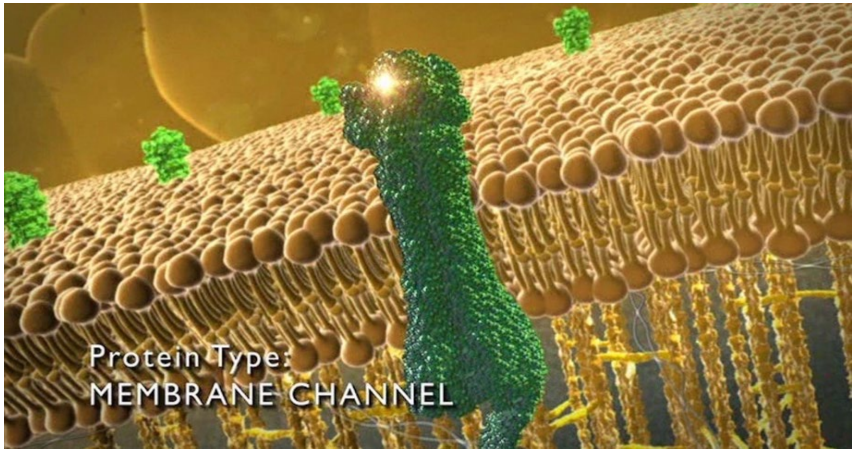
Multiscale geometry in DRACO

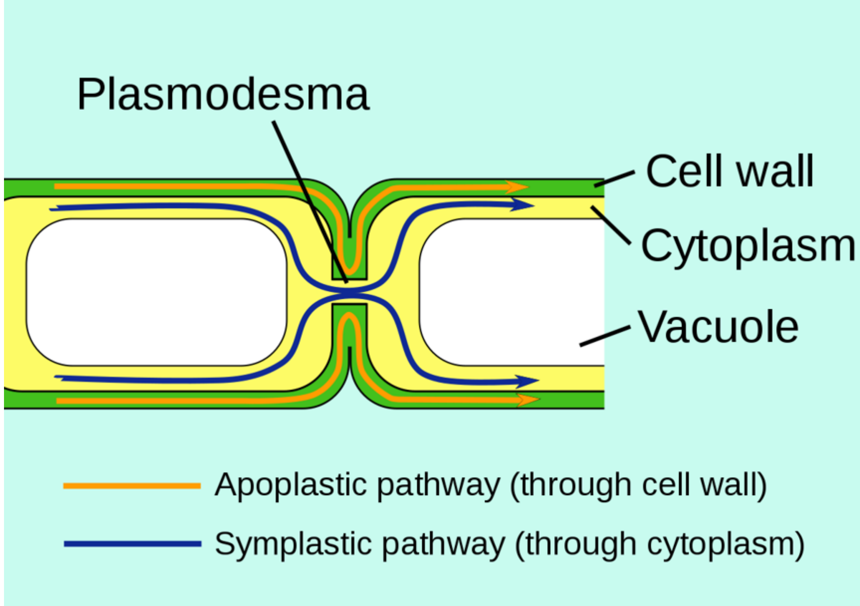




Constrained diffusion. Reactions in bulk and at surface.

Constrained transport is common in biology





Diffusion has different properties in 3D, 2D, and 1D

DRACO is the best tool when:

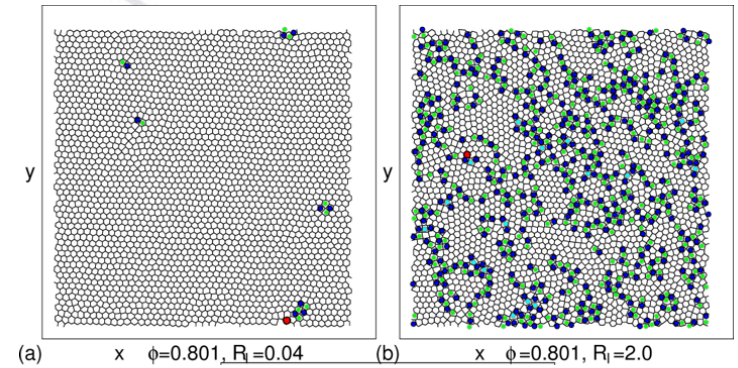
- Diffusion constrained by a complex geometry.
- Diffusion channels are much smaller than other scales in system.
- Multiple interacting gas producing and gas absorbing materials.
- Separated time scales: fast reactions, slower diffusion.
- Two diffusive time scales: surface (faster) and bulk (slower)

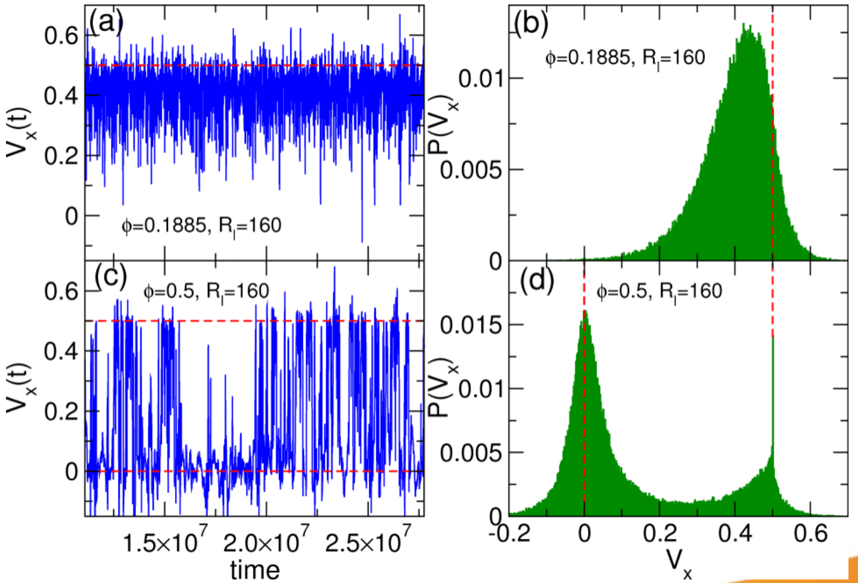
Challenges in Understanding Aging

- System is out of equilibrium so many thermodynamic concepts do not apply.
- Behavior often dominated by rare “worst case” events instead of average events (failure of central limit theorem).
- Existence of a threshold can produce very abrupt behavior change.
- Behavior depends on time history of system (lack of state variables).

Heterogeneity

- Average bulk response of material not representative of actual response inside material.
- Bulk behavior may be determined by properties of a few local areas that are especially strong or weak.
- Behavior is difficult to model and predict.

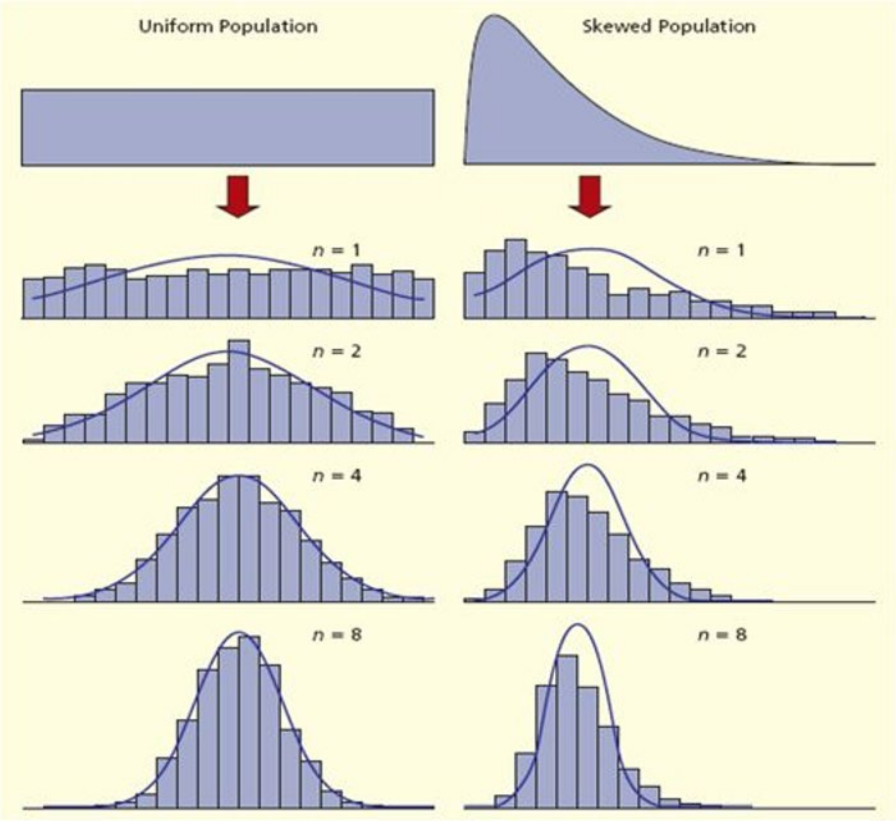




Phys. Rev. E 91, 032313 (2015)

Failure of the central limit theorem

- Typically, as the number of samples increases, behavior tends toward the average.

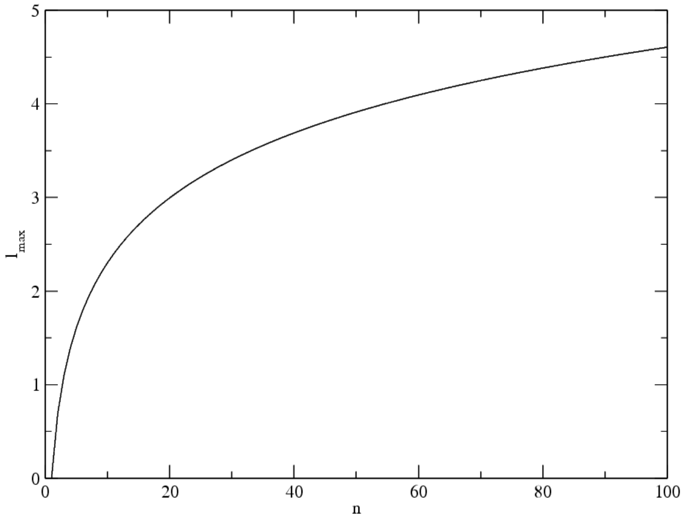


Failure of the central limit theorem

- If extreme events dominate behavior (e.g., weakest link), most extreme event becomes more extreme as number of samples increases. (Weibull)

PCO

l_{max}

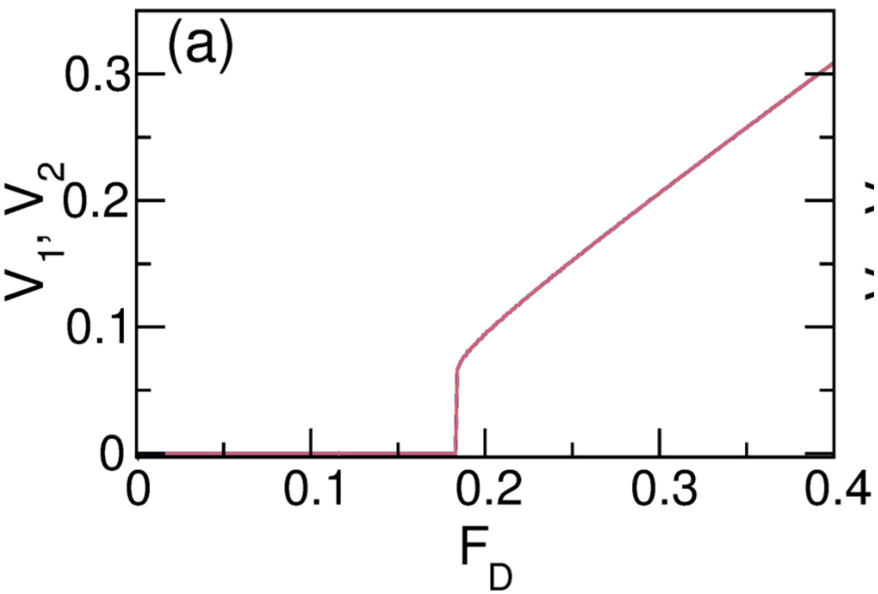


L

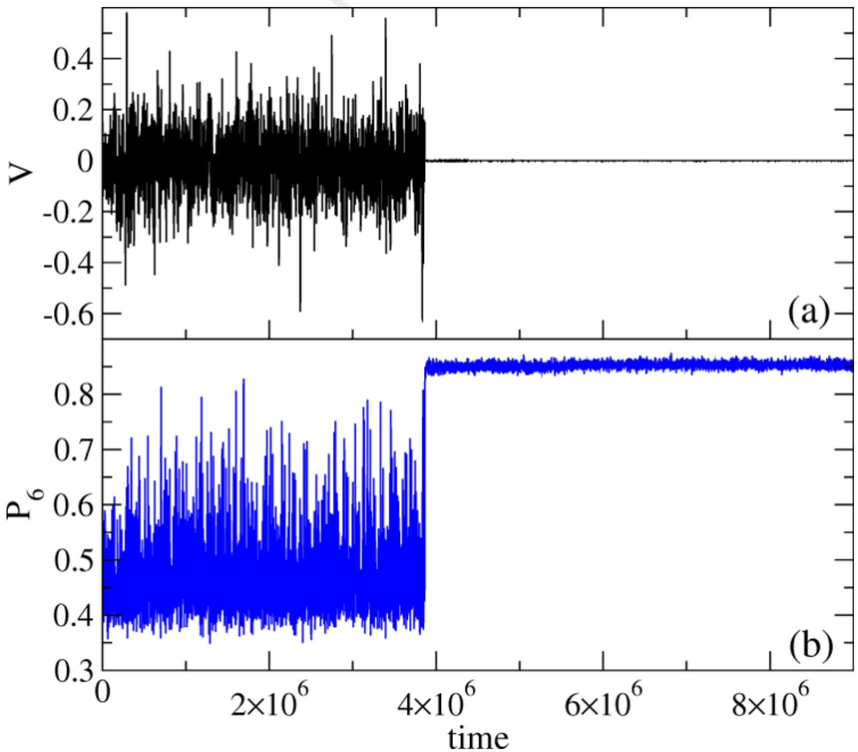
$$l_{max} = a_0 \ln n.$$

$$G_n(x) = \int_{-\infty}^{x} g_n(x)dx = 1 - (1 - F(x))^n.$$

Thresholds and transients

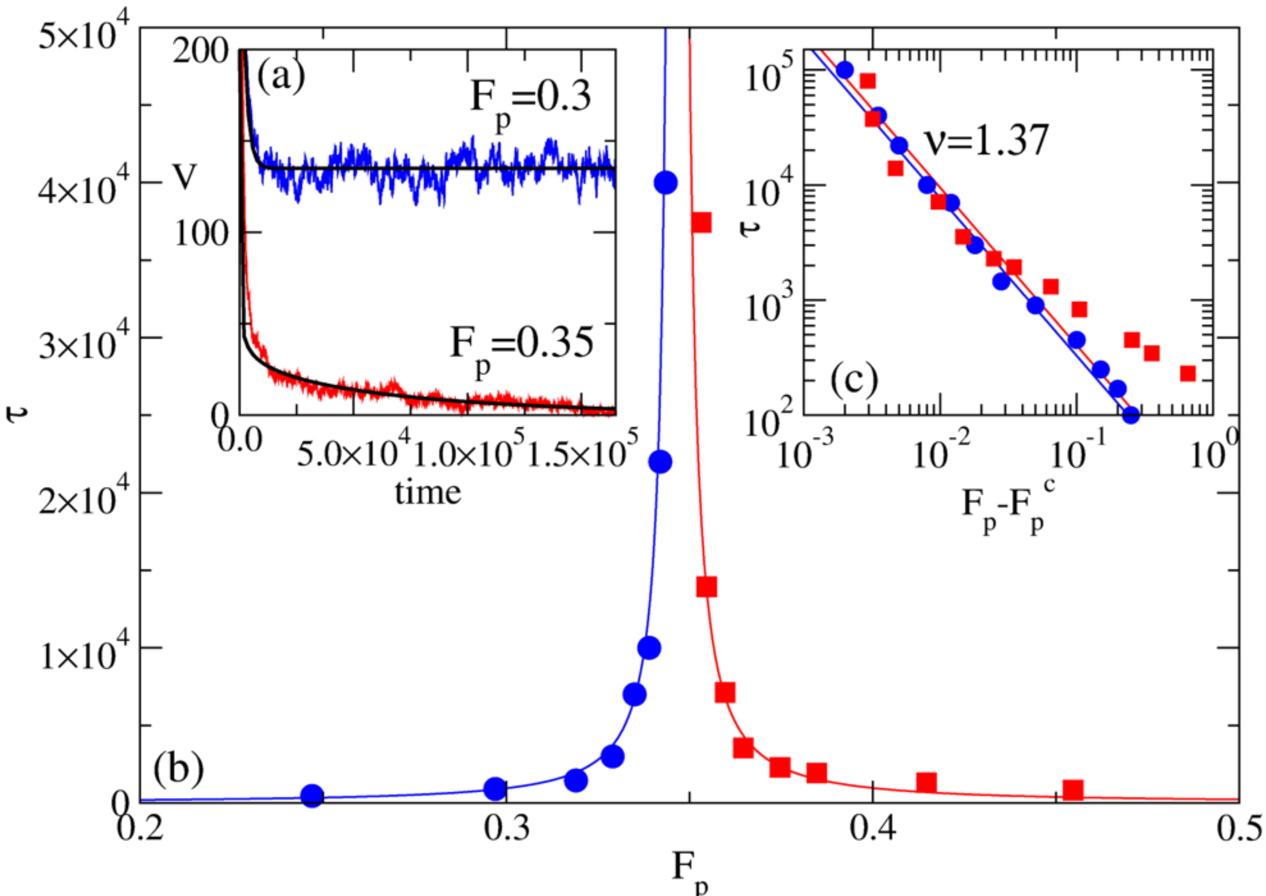


Rep. Prog. Phys. 80, 026501 (2017)



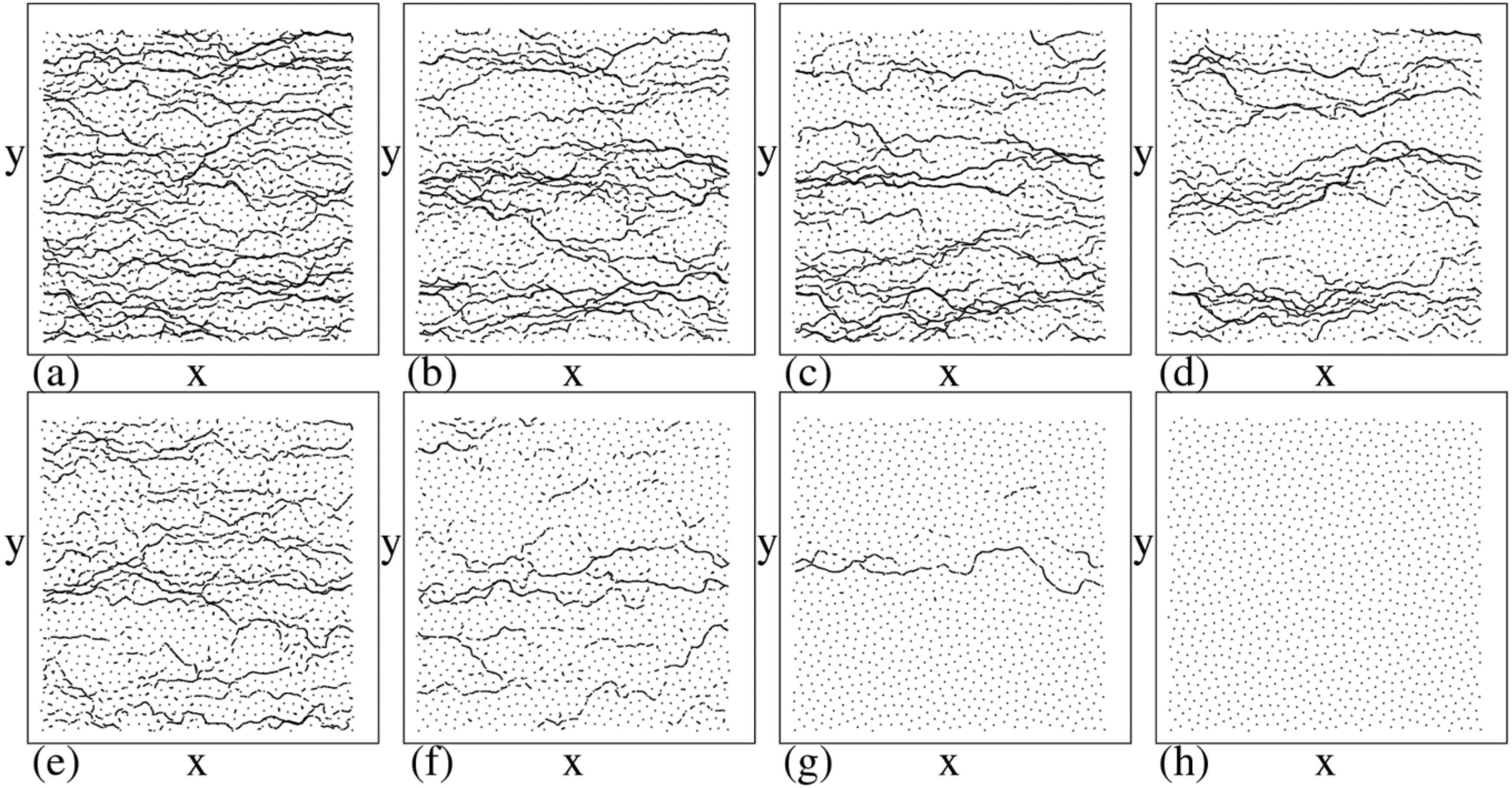
Soft Matter 10, 7502 (2014)

Diverging time scale



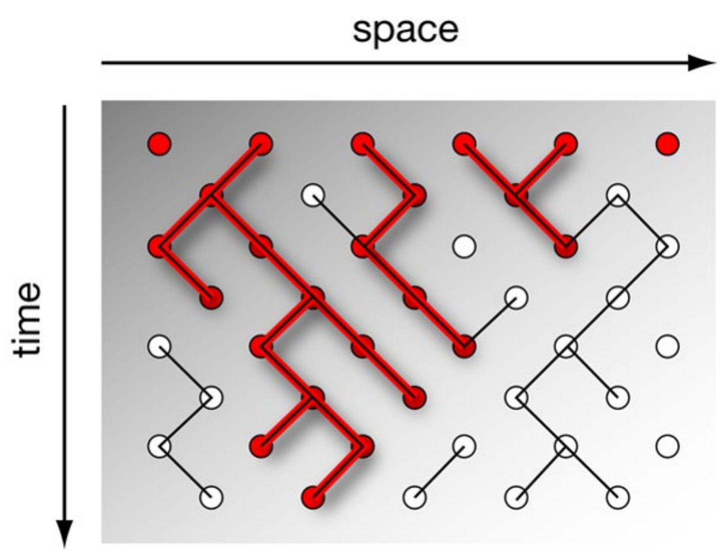
Rep. Prog. Phys. 80, 026501 (2017)

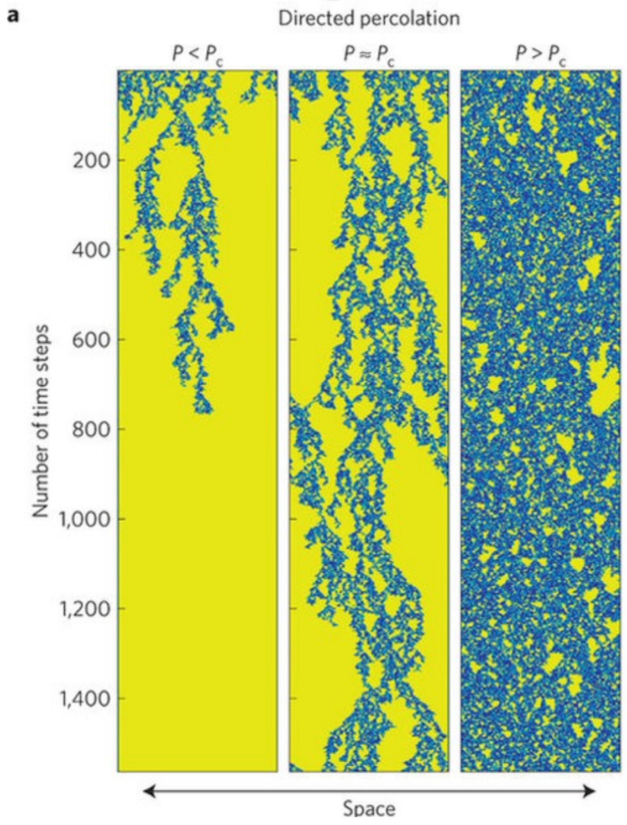
Absorbing phase transition



Phys. Rev. Lett. 103, 168301 (2009)

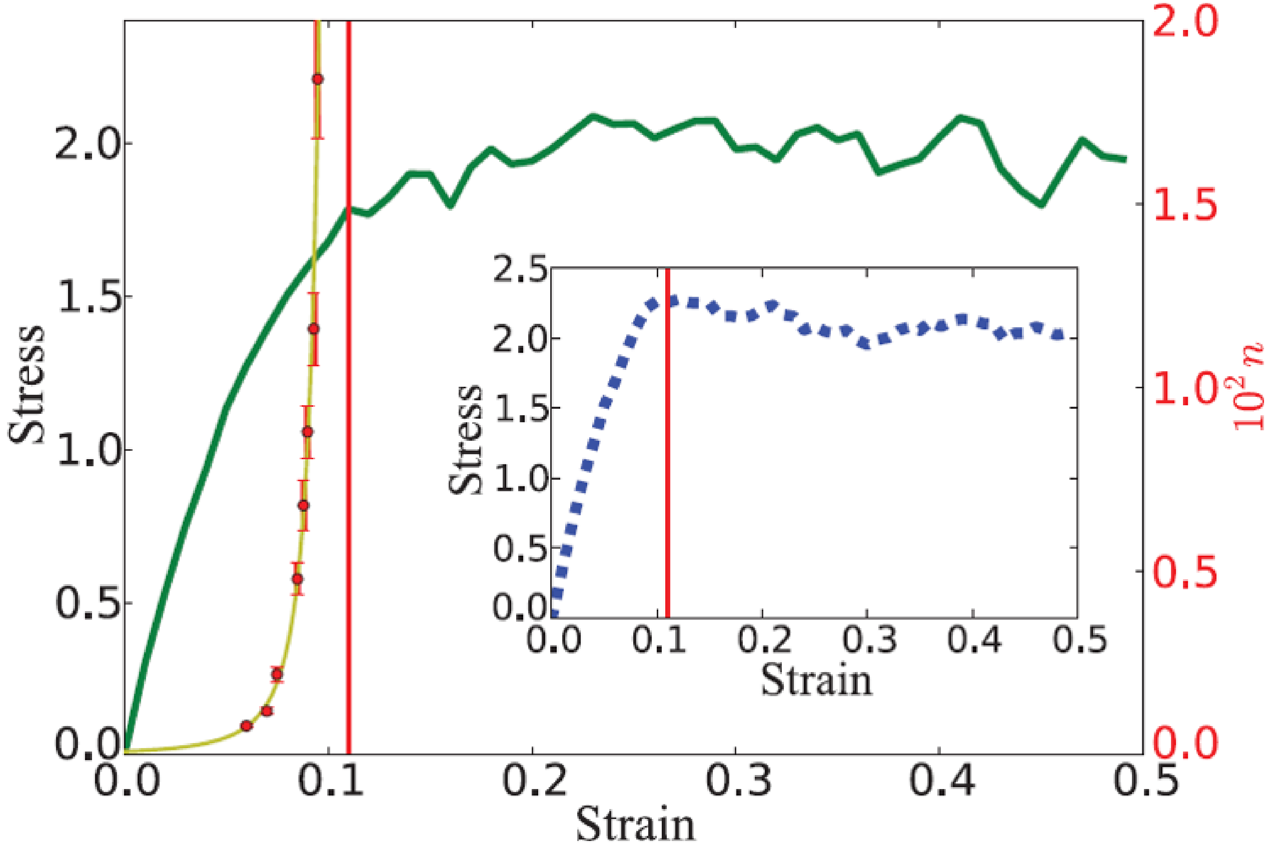
Absorbing phase transition (Directed percolation) from fluctuating to nonfluctuating state





M. Kohl et al, Nat. Commun. 7, 11817 (2016).

Absorbing phase transition in metallic glass



Rep. Prog. Phys. 80, 026501 (2017)

Summary

- DRACO designed for multi-physics reaction-diffusion when narrow channels strongly constrain gas motion.
- Tools from nonequilibrium statistical mechanics can be applied to aging problems.
- Extreme value statistics: when behavior dominated by rare events.
- Threshold processes: when sudden changes of behavior occur.
- Absorbing phase transitions: associated with diverging time scales, long transients, and strong history dependence.